KING FAHD UNIVERSITY of PETROLIUM and MINERALS
Physics Department
Atomic and Molecular Physics (Phys-551)
Spring 2014

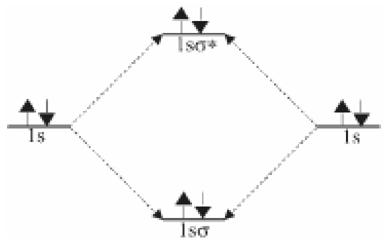
Issued: 27-2-2014	**First Test**	Time: 120 min

In the exam:

1- **Use atomic units**
2- **Write your answer on one side of the answer sheet.**
3- **Each question answer should be in separate sheets.**
4- **For the spin states, define your state as** $\left|\uparrow\uparrow\right\rangle$ **, or** $\left|+\frac{1}{2}+\frac{1}{2}\right\rangle$ **or** $\left|\alpha\alpha\right\rangle$**, for two parallel upward spin particles.**
5- **All problems have equal weight. So, it is up to you to start with the simple one.**
6- ***If your answer is yes, or no, you have to give the reason, or reasons.***

1- ***Is the helium monatomic gas***? **Yes**

Helium molecule (He_2): has four electrons, two in the bonding state $\sigma_g 1\mathrm{s}$ and two in the antibonding state $\sigma_u^* 1\mathrm{s}$; that is, $(\sigma_g 1\mathrm{s})^2\,(\sigma_u^* 1\mathrm{s})^2$



The bond order for the helium molecule is $\frac{2-2}{2}=0$, i.e. **no stable configuration is produced**, so He_2 does not exist. ***This explains why helium is a monatomic gas***.

2- Is the function $\psi(r_1,r_2)=\phi_{100}(\vec{r}_1)\ \phi_{100}(\vec{r}_2)\chi_{\text{triplet}}$ correct to describe the ground state of He-atom? **No** [χ_{triplet} is the two-particle spin triplet state,]

$\psi(r_1,r_2)$ should be antisymmetric, but both functions $\phi_{100}(\vec{r}_1)\ \phi_{100}(\vec{r}_2)$ and χ_{triplet} are symmetric.

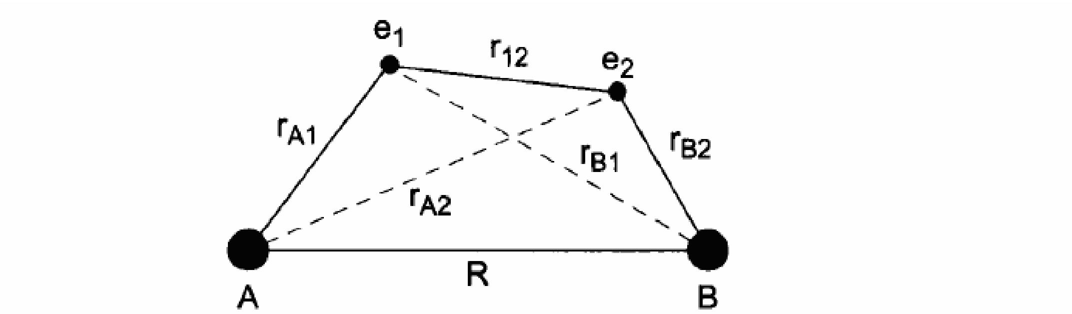
3- Is Zeeman's effect can be seen for the two electrons in the s-state? **No**

For two electrons in the s-state, one finds $m_s=0$ and $m_\ell=0$, so $\Delta E\propto(m_\ell+2m_s)=0$

4- Is the uncouple function $|\ell m_\ell\rangle|sm_s\rangle$ suitable for the perturbation $\vec{\mathrm{L}}.\vec{\mathrm{S}}$? **No**

$|\ell m_\ell\rangle|sm_s\rangle$ will not diagonalizes the term $\vec{\mathrm{L}}.\vec{\mathrm{S}}$.

5- The following figure shows the H-molecule, see; write down the **full** Hamiltonian of the system.



Schematic diagram of hydrogen molecule

Answer:

$$\hat{H} = -\frac{1}{2}\nabla_A^2 - \frac{1}{2}\nabla_B^2 + \hat{H}(1) + \hat{H}(2) + \frac{1}{r_{12}} + \frac{1}{R}$$

where

$$\hat{H}(i) = -\frac{1}{2}\nabla_e^2(i) - \frac{1}{r_{Ai}} - \frac{1}{r_{Bi}}, \qquad i = 1, 2$$

6- Use the spin wave function for an electron $\psi = a\,\alpha + b\,\beta$, where *a* and *b* are constants, to complete the following equations:

$$\hat{S}^2\psi = \frac{1}{2}\left(\frac{1}{2}+1\right)\psi = \frac{3}{4}\psi$$

$$\hat{S}_z^2\psi = \frac{1}{4}\psi$$

7- Classify each of these functions as symmetric (S), antisymmetric (A), or neither symmetric nor antisymmetric (N).

function	classification
$f(1)g(2)\alpha(1)\alpha(2)$	N
$f(1)f(2)\left[\alpha(1)\beta(2)-\alpha(2)\beta(1)\right]$	A
$f(1)f(2)f(3)\beta(1)\beta(2)\beta(3)$	S
$e^{-(r_1-r_2)}$	N
$\left[f(1)g(2)-f(2)g(1)\right]\left[\alpha(1)\beta(2)-\alpha(2)\beta(1)\right]$	S
$r_{12}^2 e^{-(r_1+r_2)}$	S

8- Two electrons, each with spin $\frac{1}{2}$, are in s-state. If the perturbation term is:

$$\hat{H}' = A\,\hat{S}_1.\hat{S}_2$$

where A is positive constant:

a- Calculate the energy eigenvalue, or eigenvalues, of the perturbation.

b- Draw a diagram showing how the energy levels of $\hat{H}'$ split.

Answer: Calculate the energy eigenvalue, or eigenvalues, of the perturbation.

$$s_1 = \frac{1}{2}, s_2 = \frac{1}{2} \Rightarrow s = 0,1$$

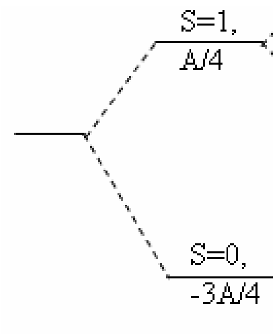
$$\hat{S}_1.\hat{S}_2 = \frac{1}{2}\left[\hat{S}^2 - \hat{S}_1^2 - \hat{S}_2^2\right]$$

$$E_1 = \langle SM_s | K\hat{S}_1.\hat{S}_2 | SM_s \rangle = \frac{A}{2}\left[s(s+1) - \frac{1}{2}(\frac{1}{2}+1) - \frac{1}{2}(\frac{1}{2}+1)\right]$$

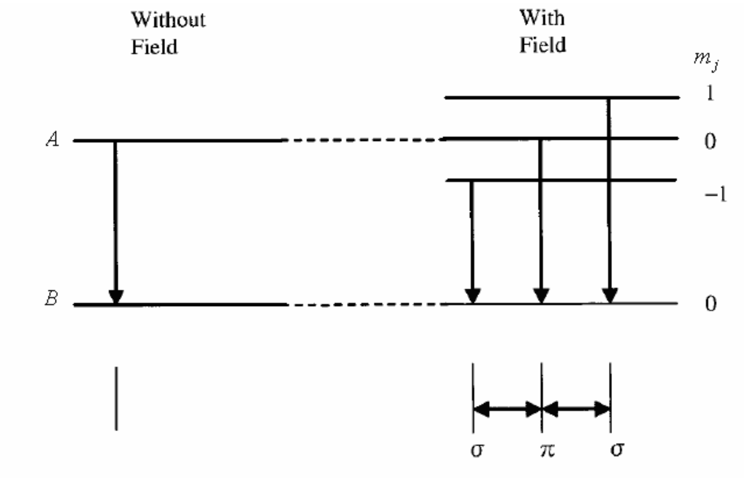
$$= \frac{A}{2}\left[s(s+1) - \frac{1}{2}(\frac{1}{2}+1) - \frac{1}{2}(\frac{1}{2}+1)\right] \quad = \frac{K}{2}\left[s(s+1) - \frac{3}{2}\right]$$

$$= A\begin{cases} \frac{1}{4} & \text{for triplet} \\ -\frac{3}{4} & \text{for singlet} \end{cases}$$

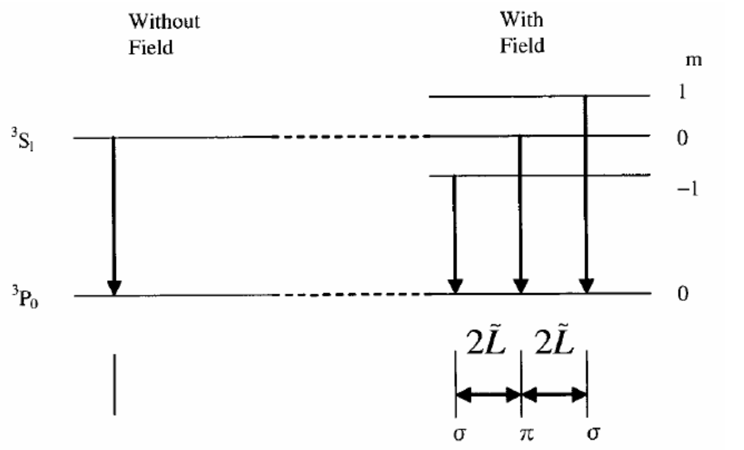
b-



9- The following figure is the transitions of anomalous Zeeman effect for of unknown states A and B. What are these states?



Answer:



Answer: $\begin{pmatrix} A \\ B \end{pmatrix} \equiv \begin{pmatrix} {}^3S_1 \\ {}^3P_0 \end{pmatrix} \equiv \begin{pmatrix} {}^1P_1 \\ {}^1S_0 \end{pmatrix}$

10- A particle of spin $\frac{1}{2}$ is in a p-sate of orbital angular momentum $(l = 1)$. Consider its perturbed Hamiltonian is given by:

$$\hat{H} = a + b\hat{L}.\hat{S} + c\hat{L}^2$$

where *a*, *b*, and *c* are constants. Find the energy values for each of the different states of the total angular momentum J. (Express your answer in terms of *a*, *b*, and *c*).

Answer:

$$\hat{H} = a + b\hat{L}.\hat{S} + c\hat{L}^2 = a + b\,\frac{(\hat{J}^2 - \hat{L}^2 - \hat{S}^2)}{2} + c\hat{L}^2$$

$$J = \frac{1}{2}, \frac{3}{2}$$

$$\hat{\vec{L}}.\hat{\vec{S}}\left|\ell, s, j, m_j\right\rangle = \frac{1}{2}\left(\hat{J}^2 - \hat{L}^2 - \hat{S}^2\right)\left|\ell, s, j, m_j\right\rangle$$

$$= \frac{1}{2}\left[j(j+1) - \ell(\ell+1) - s(s+1)\right]\left|\ell, s, j, m_j\right\rangle$$

$$\left\langle \hat{L}^2 \right\rangle = \ell\left(\ell + 1\right)$$

$$\left\langle \hat{\vec{L}}.\hat{\vec{S}} \right\rangle = \left\langle l, s, j, m_j \left| \hat{\vec{L}}.\hat{\vec{S}} \right| l, s, j, m_j \right\rangle = \frac{\hbar^2}{2}\left[j(j+1) - l(l+1) - \frac{3}{4}\right]$$

$$\left\langle \hat{H} \right\rangle = a + b\left\langle \hat{L}.\hat{S} \right\rangle + c\left\langle \hat{L}^2 \right\rangle = a + b\,\frac{1}{2}\left[j(j+1) - \ell(\ell+1) - \frac{3}{4}\right] + c\,\ell\left(\ell+1\right)$$

$$E_{j=1/2} = \left\langle \hat{H} \right\rangle_{j=1/2} = a + b\,\frac{1}{2}\left[\frac{1}{2}(\frac{1}{2}+1) - 1(1+1) - \frac{3}{4}\right] + c1\left(1+1\right)$$

$$= a + \frac{b}{2}\left[-2\right] + 2c = a - b + 2c$$

$$E_{j=3/2} = \left\langle \hat{H} \right\rangle_{j=3/2} = a + b\,\frac{1}{2}\left[\frac{3}{2}(\frac{3}{2}+1) - 1(1+1) - \frac{3}{4}\right] + c1\left(1+1\right)$$

$$= a + \frac{b}{2}\left[1\right] + 2c = a + \frac{b}{2} + 2c$$

11- For an electron in P-state, calculate:

$$\vec{L}\cdot\vec{S}\left|m_\ell=0,m_s=\frac{1}{2}\right\rangle \text{, hence find } \left\langle 0,\frac{1}{2}\right|\vec{L}\cdot\vec{S}\left|0,\frac{1}{2}\right\rangle \text{ and } \left\langle 1,-\frac{1}{2}\right|\vec{L}\cdot\vec{S}\left|0,\frac{1}{2}\right\rangle$$

Answer:

$$\vec{L}\cdot\vec{S}\left|0,\frac{1}{2}\right\rangle=\hat{L}_z\hat{S}_z\left|0,\frac{1}{2}\right\rangle+\frac{1}{2}\left(\hat{L}_+\hat{S}_-+\hat{L}_-\hat{S}_+\right)\left|0,\frac{1}{2}\right\rangle$$

$$\hat{L}_z\hat{S}_z\left|0,\frac{1}{2}\right\rangle=\hat{L}_z\left(\hat{S}_z\left|0,\frac{1}{2}\right\rangle\right)=\frac{1}{2}\left(\hat{L}_z\left|0,\frac{3}{2}\right\rangle\right)=\frac{1}{2}\times 0\times\left|1,\frac{3}{2}\right\rangle=0,$$

$$\frac{1}{2}\left(\hat{L}_+\hat{S}_-\right)\left|0,\frac{1}{2}\right\rangle=\frac{1}{2}\hat{L}_+\left(\hat{S}_-\left|0,\frac{1}{2}\right\rangle\right)=\sqrt{\frac{1}{2}(\frac{1}{2}+1)-\frac{1}{2}(\frac{1}{2}-1)}\left(\frac{1}{2}\hat{L}_+\left|0,-\frac{1}{2}\right\rangle\right)=\frac{1}{2}\hat{L}_+\left|0,-\frac{1}{2}\right\rangle$$

$$=\frac{1}{2}\sqrt{1(1+1)-0(0+1)}\left|1,-\frac{1}{2}\right\rangle=\frac{1}{2}\sqrt{2}\left|1,-\frac{1}{2}\right\rangle,$$

$$\frac{1}{2}\left(\hat{L}_-\hat{S}_+\right)\left|0,\frac{1}{2}\right\rangle=\frac{1}{2}\sqrt{1(1+1)-0(0-1)}\sqrt{\frac{1}{2}(\frac{1}{2}+1)-\frac{1}{2}(\frac{1}{2}+1)}\left|-1,\frac{3}{2}\right\rangle=0$$

Then:

$$\left\langle m_l,m_s\right|\vec{L}\cdot\vec{S}\left|0,\frac{1}{2}\right\rangle=\frac{1}{\sqrt{2}}\left\langle m_l,m_s\right|\left|1,-\frac{1}{2}\right\rangle=\frac{1}{\sqrt{2}}\delta_{m_l,1}\delta_{m_s,-\frac{1}{2}}$$

$$\left\langle 0,\frac{1}{2}\right|\vec{L}\cdot\vec{S}\left|0,\frac{1}{2}\right\rangle=0,$$

$$\left\langle 1,-\frac{1}{2}\right|\vec{L}\cdot\vec{S}\left|0,\frac{1}{2}\right\rangle=\frac{1}{\sqrt{2}}$$

12- For the coupling of two non equivalent electrons $np\ n'p$, the relation between the coupled and uncoupled for the upper states are given by:

$$\left|22\right\rangle=\left|11\right\rangle$$

$$\left|21\right\rangle=\frac{1}{\sqrt{2}}\left|10\right\rangle+\frac{1}{\sqrt{2}}\left|01\right\rangle$$

Calculate the next lower state.

Answer: $\left|20\right\rangle=\frac{1}{\sqrt{6}}\left|1-1\right\rangle+\sqrt{\frac{2}{3}}\left|00\right\rangle+\frac{1}{\sqrt{6}}\left|-11\right\rangle$

13- An electron in the state $\left|n,\ell,s,j,m_j\right\rangle$ with $n=5$. Use this information to:

a. Write down the ℓ values

Answer: $\ell = 0,1,2,3,4$

b. Write down the highest state in the couple representation, i.e. $\left|n,\ell,s,j,m_j\right\rangle$.

Answer: $\left|\ell,s,j,m_j\right\rangle = \left|4,\frac{1}{2},\frac{9}{2},\frac{9}{2}\right\rangle$.

c. Write down the highest state in the uncouple representation, i.e. $\left|\ell,m_\ell,s,m_s\right\rangle$.

Answer: $\left|\ell,m_\ell,s,m_s\right\rangle = \left|4,4,\frac{1}{2},\frac{1}{2}\right\rangle$.

d. Use the lowering operator technique to calculate the next couple representation of the results in part a in terms of the uncouple representation.

Answer: $\left|4,\frac{1}{2},\frac{9}{2},\frac{7}{2}\right\rangle = \frac{1}{3}\left|4,4,\frac{1}{2},-\frac{1}{2}\right\rangle + \frac{\sqrt{8}}{3}\left|4,3,\frac{1}{2},\frac{1}{2}\right\rangle$.

14- For two identical fermions in different states designated by $n\ell$ and $n'\ell'$, the expectation term of $\frac{1}{r_{12}}$ is given by:

$$\left\langle \frac{1}{r_{12}} \right\rangle = J \pm K$$

Write J and K in terms of the wave functions of the two particles.

Answer:

$$J = \int\int d\tau_1 d\tau_2 \, \frac{\left|\psi_\ell(1)\right|^2 \left|\psi_{\ell'}(2)\right|^2}{r_{12}}, \qquad K = \int\int d\tau_1 d\tau_2 \, \psi_\ell^*(1)\psi_{\ell'}(1)\frac{1}{r_{12}}\psi_{\ell'}^*(2)\psi_\ell(2)$$

14- Assuming the $\hat{L}.\hat{S}$ interaction to be much stronger than the interaction with an external magnetic field, calculate the anomalous Zeeman splitting of the lowest states $\left({}^2S_{1/2},\ {}^2P_{1/2},\ {}^2P_{3/2}\right)$ in Hydrogen for a field of 0.05 T.

Answer:

$$\Delta E = H_m = \beta(\vec{L} + 2\vec{S})\cdot\vec{B} = \beta g_J m_J B = \beta\left\{1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}\right\} m_J B$$

$$= \left(5.788\times10^{-5}\ \frac{\text{eV}}{\text{T}}\right) g_J (0.05\ \text{T}) m_J$$

With

$$g_J = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

State	L	S	J (M_J)	g	ΔE (eV)$\times10^{-5}$
${}^2P_{3/2}$	1	1/2	3/2 ($\pm3/2$, $\pm1/2$)	4/3	±0.579 ±0.193
${}^2P_{1/2}$	1	1/2	1/2 ($\pm1/2$)	2/3	±0.097
${}^2S_{1/2}$	0	1/2	1/2 ($\pm1/2$)	2	±0.290